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CONCAVE PROGRAMMING FOR GASOLINE BLENDING

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CONCAVE PROGRAMMING FOR GASOLINE BLENDS [1]

A. S. Manne

1. Introduction

This paper presents a model of the economics of motor gasoline blending -- a maximizing problem subject to certain restraints. The computation of the model cannot be handled within the framework of conventional Lagrangean multipliers. As yet, neither George Dantzig nor I have succeeded in converting the system into a linear programming setup that is short enough to be convenient for computational purposes, and which at the same time preserves the octane technology.

Kuhn and Tucker [7] have established the theorem that a solution to this type of maximizing problem is equivalent to a certain minimax saddlepoint, and at the suggestion of Harry Markowitz, the gasoline blending model was recast into the appropriate minimax form. An iterative digital technique was then devised for solving the minimax problem. [2]

From a rigorous mathematical standpoint, the present iterative technique is by no means satisfactory. The method does, however, lead to solutions that should be sufficiently accurate from the standpoint of refinery managers. Convergence takes place without an inordinate amount of computing time. All calculations were performed on a machine that is readily available throughout the United States -- an IBM Card

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Programmed Calculator, Model 2. A general purpose floating decimal setup
was employed. On the first problem run off, approximately ten hours of
running time were required. For the sixth problem of this type, the running
time had been cut down to less than three hours.

In order to maintain a check on the solutions, the model was kept simple
enough so that it could also be solved by graphical techniques. For that
reason, the model will not in itself be of interest to refinery operators.
From their standpoint, nevertheless, the computations are significant. The
results bring into question the validity of a number of rules-of-thumb that
are current in the industry for solving this type of economic problem. A
second point: the calculations give some indication of the financial improve-
ment that may be obtained by taking account of non-linear octane blending
relationships. And finally, these machine runs have served as a pilot study,
preliminary to attacking problems that involve larger numbers of variables.

The material will be presented in the following sequence: octane number
prediction devices; the economic model; the computational procedure; and then
a discussion of the results of the six CPC runs.

2. Octane number predictions

Like most kinds of engineering work, the forecast of gasoline octane
numbers is more of an art than an exact science. Refiners themselves neces-
sarily make paper forecasts of the octane number of proposed blends, but before
marketing a product they will almost inevitably take the precaution of testing
the mixture in an octane rating engine.

(a) Tetraethyl lead concentration levels.

One phase of the problem has been investigated extensively by the refining
industry -- the relationship between octane numbers and the amount of tetraethyl
lead added per gallon of a particular gasoline. It has been invariably observed
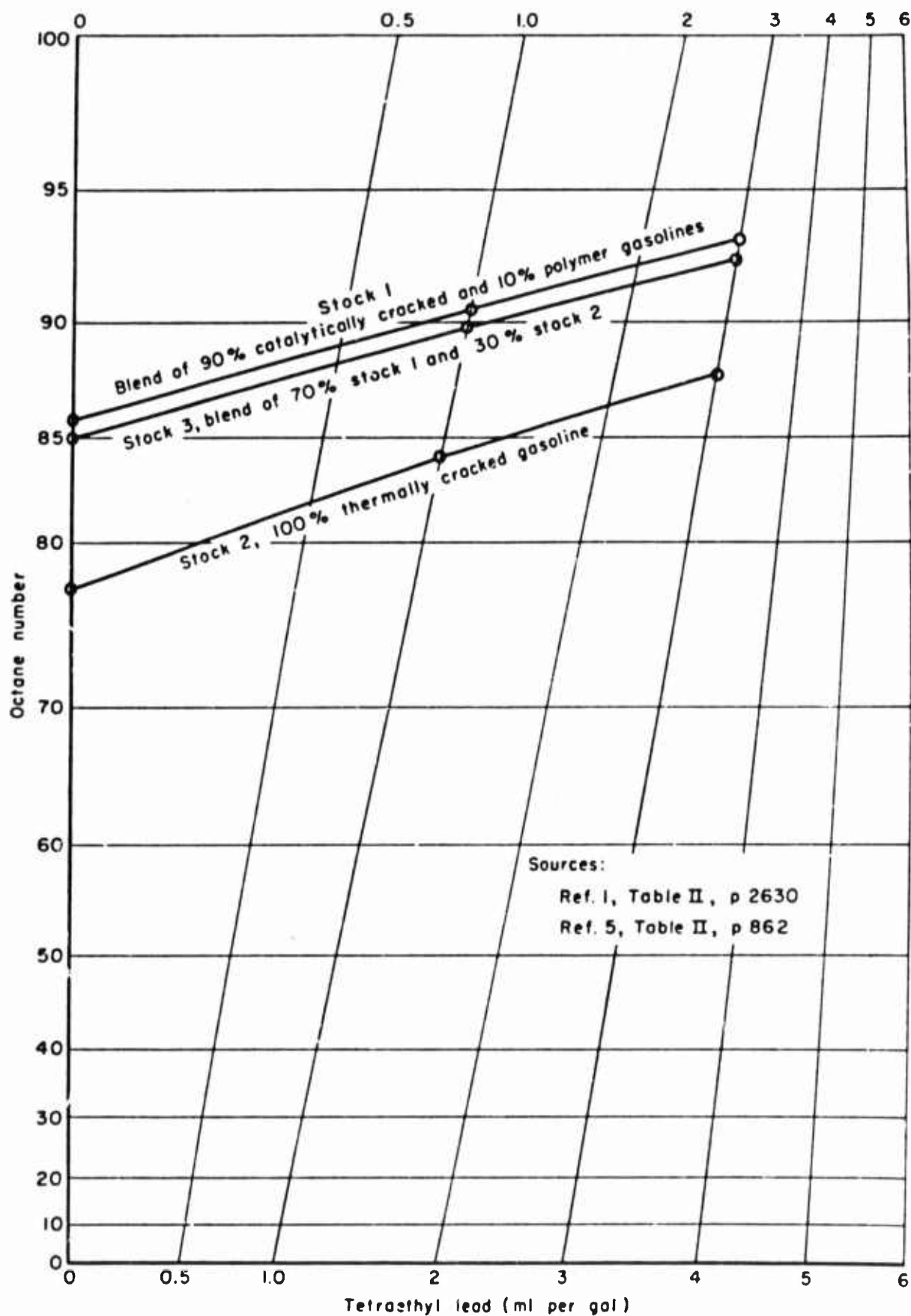
Fig. 1—Octane number versus TEL concentration for three gasolines

that, as the lead concentration level is increased, the octane number increases at a decreasing rate. In order to predict this relationship, there is in widespread use an ethyl blending nomogram, reproduced as Figure 1. The points obtained by testing a particular gasoline, when plotted on such charts, will generally lie along a straight line. The line labelled "1" represents three observations for a particular gasoline reported by Bogen and Nichols.[1] The lines labelled "2" and "3" represent two more sets of observations reported by them. In order to cut down on the number of knock engine runs, it is the general practice to test one sample of clear gasoline (i.e., no TEL) and another sample of the same gasoline containing 3 ml. of the ethyl fluid. (3 ml. typically represents the maximum allowable concentration in American motor gasolines.) These tests yield two points which can be plotted on the blending paper. The octane numbers for intermediate lead concentration levels can then be predicted by straight line interpolation.

The ethyl blending chart that is in general use -- the one put forward by Hebl, Rendel, and Garton in 1939 [5] -- was itself derived from empirical observations, and not from any algebraic formula. I have found, however, that there is a three-parameter analytic expression that gives a close approximation to the results predicted by the blending chart. Where t represents the octane number of the leaded gasoline, and x represents the TEL concentration level (in ml. per gallon):

$$(1) \qquad t = a + bx + \frac{c}{1 + x}$$

For any unknown gasoline, the three parameters, a, b, and c, have to be determined. This may be accomplished readily by taking three

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[1] [1, Table 2, p. 2630.]

observations of octane number for various lead levels, and solving three simul-
taneous linear equations. Two observations can be the experimental ones, and
the third may be determined in the standard way on the ethyl blending chart.
Using equation (1) in this way, approximately 20 sets of constants have been
determined for actual gasolines. Testing seven lead levels in each of these 20
cases, the equation has virtually always given a prediction that lies within $\pm$
0.2 octane number of the one yielded by the blending chart.

No special significance should be attached to the particular form of equation
(1). It is merely a device for enabling a computing machine to perform the same
calculation as a refiner with his blending chart and his straight edge.

(b) Two-component gasoline blends.

A second phase of the blending problem is more controversial than the TEL
aspect. For a lead level of, say, 3 ml., and for a 50-50 mixture of two gas-
olines A and B, refiners frequently calculate the octane number of the blend
to be the 50-50 weighted average of the octane number of gasolines A and B —
each with 3 ml. The weighted average appears satisfactory for many gasolines —
especially when both components are of paraffinic nature. There are, however,
at least two papers publicly available -- one by Eastman $/ L /$ and the other
by Bogen and Nichols $/ 1 /$ -- that call into question the straight-line averag-
ing method. Both papers indicate that as the percentage of the high octane
component in a binary mixture increases (both components initially at the same
TEL concentration level), the octane level of the mixture may increase at a
decreasing rate. Geometrically, the octane number is a concave, monotone-
increasing function of the percentage of the high-octane component in the
blend. In ordinary language, the octane number of the blend tends to exceed
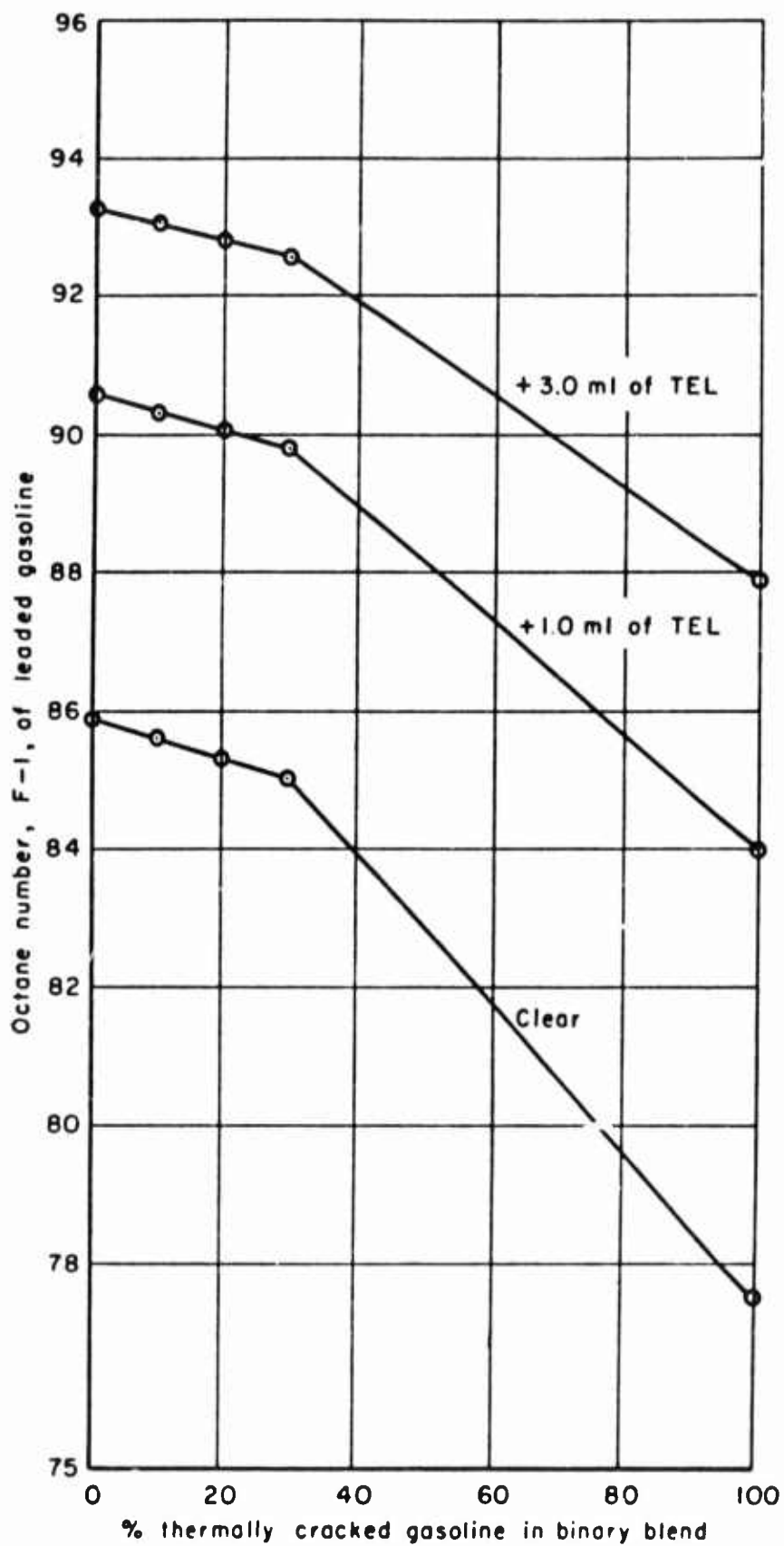the weighted average of the octane number of the two components.

Fig. 2—Octane number versus percent of thermally cracked component in binary blend. Three TEL levels

Bogen and Nichols are primarily concerned with three-component mixtures, and they report only five observations at each of three TEL levels for strictly binary mixtures. The set of 15 points has been plotted, and is reproduced as Figure 2. These 15 observations are the basis for constructing the present model. For each TEL concentration level shown on this chart, straight-line interpolation has been used between adjacent observations. In all likelihood, these straight lines also underestimate the octane number that is attainable by blending. The existing data, unfortunately, do not provide a basis for curvilinear interpolation.

At first glance, it would appear to be a trivial matter whether octane numbers were calculated by drawing straight lines between two adjacent points or between two end points of a constant-TEL line. Nevertheless, a sample calculation presented below in Section (6) indicates that the two methods lead to TEL input requirements that differ by 20%!

3. An economic model of the blending problem

It is assumed that the refiner has available fixed quantities, q_1 and q_2, of two blendings stocks - of types 1 and 2, respectively. The #1 stock is the high octane, catalytic-cracked-plus-polymer gasoline, tested by Bogen and Nichols. The #2 stock is their low octane, thermally cracked gasoline. These two may be blended together in any proportions, and may be mixed with tetraethyl lead. There are two products -- 1 and 2 -- premium and regular grade gasoline, respectively. These two are to meet minimum F-1 (Research) octane number specifications of N_1 and N_2, and they may be sold at unit prices, p_1 and p_2. The cost of 1 ml. of tetraethyl lead is represented by p_3.

Instead of using the two blending stocks directly for producing finished gasoline, the refiner may also elect to produce a fictitious

intermediate product - "stock 3" - by mixing together the two initial materials in 70-30 proportions. This third stock may in turn be blended into either of the two finished products. By permitting the refiner to produce this fictitious intermediate product, the model in effect permits him to interpolate between all adjacent observations on Chart 2. There are eight independent variables in the problem, x_i, defined as follows:

$$(2) \qquad x_{11} = \text{number of gallons of stock 1 in product 1}$$

$$x_{21} = \text{number of gallons of stock 2 in product 1}$$

$$x_{31} = \text{number of gallons of stock 3 in product 1}$$

$$x_{41} = \text{ml. of tetraethyl lead per gallon of product 1}$$

$$x_{12} = \text{number of gallons of stock 1 in product 2}$$

$$x_{22} = \text{number of gallons of stock 2 in product 2}$$

$$x_{32} = \text{number of gallons of stock 3 in product 2}$$

$$x_{42} = \text{ml. of tetraethyl lead per gallon of product 2}$$

The set of 8 x_i will be indicated by the vector $\underline{x}$. The refinery's net gasoline realization will be termed $g(x)$. The net realization on one gallon of product equals the selling price of that product, less the TEL cost per gallon.

$$(3) \qquad g(x) = (p_1 - p_3 x_{41})(x_{11} + x_{21} + x_{31})$$
$$+ (p_2 - p_3 x_{42})(x_{12} + x_{22} + x_{32})$$

The expression for $g(x)$ is to be maximized, subject to certain restrictions, indicated below by (4) - (7), (9), and (10). The first condition is that the x_i must not be negative:

$$(4) \qquad x_i \geq 0 \qquad \qquad \text{for all } \underline{i}$$

Next, the TEL concentration levels must not exceed 3 ml. per gallon.

$$(5) \qquad 3 - x_{4j} \geq 0 \qquad\qquad j = 1, 2$$

The blending schedule, i.e. the vector $\underline{x}$, must not call for more of the blending stocks than the quantities of them that are available. The excess quantity, if any, of blending stock 1 will be denoted by f_1, and the excess of blending stock 2 by f_2.

$$(6) \qquad f_1(x) = q_1 - x_{11} - x_{12} - 0.7(x_{31} + x_{32}) \geq 0$$

$$(7) \qquad f_2(x) = q_2 - x_{21} - x_{22} - 0.3(x_{31} + x_{32}) \geq 0$$

Finally, the two gasoline products must meet the appropriate octane number specifications. To simplify the notation, a new variable is defined, t_{ij}. This variable indicates the number of octane points by which stock $\underline{i}$ exceeds (algebraically) the specifications for product $\underline{j}$, when x_{4j} ml. of lead are added to stock $\underline{i}$. The variable t_{ij} is evidently a function of x_{4j}, and is determined through the following relation:

$$(8) \qquad t_{ij}(x_{4j}) = a_i + b_i\, x_{4j} + \frac{c_i}{1 + x_{4j}} - N_j$$

In order to ensure meeting octane number specifications, the following conditions must then apply:

$$(9) \qquad f_3 = x_{11}\cdot t_{11}(x_{41}) + x_{21}\cdot t_{21}(x_{41}) + x_{31}\cdot t_{31}(x_{41}) \geq 0$$

$$(10) \qquad f_4 = x_{12}\cdot t_{12}(x_{42}) + x_{22}\cdot t_{22}(x_{42}) + x_{32}\cdot t_{32}(x_{42}) \geq 0$$

The mathematical problem posed here is the maximization of expression (3), subject to conditions (4)-(7),(9), and (10). Before going on to the computational procedure, it is worthwhile to reexamine some of the assumptions that have been slipped into the analysis.

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With the exception of the octane blending relationships, these assump-
tions closely resemble the ones underlying the avgas linear programming
model of Charnes, Cooper, and Mellon $\underline{/2\_7}$. Like the earlier model, I have
assumed that the quantities of blending stocks available and that the octane
characteristics of these blending stocks are independent of decisions in
the blending department. In fact, from the viewpoint of a refinery super-
intendent, these quantities and characteristics are·variables subject to
control. By altering the reactor temperatures, the recycle ratios, and
the assignment of intermediate distillate oil streams, the central management
is able to influence the size and composition of the gasoline blending materials
This type of interlock can only be studied in a larger model that cuts across
departmental lines.

Again, like the linear programming system, the present one assumes that
unlimited quantities of tetraethyl lead may be purchased at the going rate,
and that unlimited quantities of premium and of regular grade gasoline may
be marketed at the current spot price. Such assumptions are probably real-
istic for the smaller refiners, but they are open to serious doubt in the
case of the major ones. For the latter, a more complex type of $g(x)$ payoff
function is certainly in order. Lacking this more complex function, I have
fallen back on the simpler one. The economist can at least comfort himself
with the thought that equation (3) is the one usually employed by individual
departments within a large refining organization.

In one respect, the model at hand is less complex than the one developed
by Charnes, Cooper, and Mellon. Theirs includes a maximum vapor pressure
specification, as well as the minimum octane condition $\underline{/2}$, pp. 138-141$\_7$.
In future work, the concave programming model will be expanded to incorporate
additional restrictions of this nature. Since these other properties blend

linearly, they can be included without a large increase in the time
required for computing.

4. The computational procedure

Kuhn and Tucker have proved the following "equivalence theorem":

"Let the functions $f_1(x)$, . . . $f_m(x)$, $g(x)$ be concave as
well as differentiable for $x \geq 0$. Then x^o is a solution
of the maximum problem if, and only if, x^o and some u^o give
a solution of the saddle value problem for $\phi(x,u) \equiv g(x) +$
$u'Fx$." [1]

For the gasoline blending case, $g(x)$ is given by equation (3)
above, and the $f_j(x)$ by (6), (7), (9), and (10). The reader can verify
for himself that all these expressions are differentiable, and that (3),
(6), and (7) are concave. Furthermore, (9) and (10) will be concave over
the range $0 \leq x_{4j} \leq 3$. In other words, if we have the answer to the
problem of minimaxing $\phi(x,u)$, we also have the answer to the problem of
maximizing (3), subject to restraints (4), (5), (6), (7), (9), and (10).
The computational problem is that of finding a minimax for $\phi(x,u)$. [2]

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[1] /_7, p. 486_/ The expression $u'Fx$ is shorthand for the following:
$u_1 f_1(x) + u_2 f_2(x) + ... + u_m f_m(x)$. The u_i are non-negative
Lagrangean multipliers, and correspond closely to the economist's
notion of "shadow prices".

[2] Note that in the present version, there are not only lower limits on
the individual x_i imposed by expression (4), but also upper limits on
the x_{4j}, determined by (5). For computational purposes, it was easier
to impose these upper limits, rather than to set up additional $f_j(x)$
restrictions. The upper limits make no essential difference in the
applicability of the Kuhn-Tucker theorem.

The computational procedure is an iterative one, at each step t, converting a vector $x(t)$, $u(t)$ into a new vector $x(t + 1)$ and $u(t + 1)$. The solutions observed have tended toward the minimax point, but I can give no strict proof of the necessity of this convergence. The new vector generated is not necessarily "attainable", nor is it usually "efficient" in the sense of Koopmans $\underline{/} 6$, p. 79 $\underline{\,/}$. "Profits" do not increase monotonically as they do at each step of Dantzig's simplex procedure for linear programming $\underline{/} 3\underline{\,/}$. Despite these apparent shortcomings, the algorithm gives useful answers in the cases examined to date.

The solution must be started off from some initial vector $x(0)$, $u(0)$. In principle, this may be any arbitrary non-negative vector. In practice, though, there will be a considerable reduction in computing time if a "good" initial position is selected. At each step, first the $\underline{u}$ vector is determined, an: then the $\underline{x}$ vector. For the former, the basic iteration consists of two steps, and for the latter, of four steps. The problem is one of determining $\wedge u_j \equiv u(t + 1) - u(t)$, and $\Delta x_i \equiv x_i(t + 1) - x_i(t)$. The procedure looks cumbersome, but less than two minutes of machine time are required for generating the whole set of Δu_j and Δx_i. For the Δu_j, the procedure is as follows:

1. If $\dfrac{\partial \phi(t)}{\partial u_j(t)} \geq 0$, then the "candidate" $\widehat{\Delta u_j} = -k_j$

   If $\dfrac{\partial \phi(t)}{\partial u_j(t)} < 0$, then the "candidate" $\widehat{\Delta u_j} = k_j$

Note: k_j is an arbitrary positive constant.

2. If $u_j(t) + \widehat{\Delta u_j} < 0$, then $\Delta u_j = -u_j(t)$

   If $u_j(t) + \Delta u_j \geq 0$, then $\Delta u_j = \widehat{u_j(t)}$

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For the Δx_i, the procedure becomes:

1. If, for any j, $f_j(t) < 0$, and if $\left[\dfrac{\partial \phi(t)}{\partial x_i(t)} \cdot \dfrac{\partial f_j(t)}{\partial x_i(t)} \right] < 0$, then

    $\Delta x_i = 0$; proceed to evaluate Δx_{i+1}. Otherwise, proceed to step 2.

2. If $\dfrac{\partial \phi(t)}{\partial x_i(t)} \geq 0$, then the "candidate" $\widehat{\Delta x_i} = k_i$

    If $\dfrac{\partial \phi(t)}{\partial x_i(t)} < 0$, then the "candidate" $x_i = -k_i$

    Note: k_i is an arbitrary positive constant.

3. If $x_i't) + \widehat{\wedge x_i} < 0$, then $\Delta x_i = -x_i(t)$; proceed to evaluate x_{i+1}.

    If $x_i(t) + \widehat{\Delta x_i} \geq 0$, then proceed to step 4.

4. If $\underline{i} \neq 41$, and if $i \neq 42$, $\Delta x_i = \widehat{\wedge x_i}$; proceed to evaluate x_{i+1}.

    If $\underline{i} = 41$, or if $\underline{i} = 42$, calculate $3 - x_{4j}(t) - \widehat{\wedge x_{4j}}$.
    If this expression is non-negative, $\Delta x_{4j} = \widehat{\wedge x_{4j}}$. Otherwise,
    $\Delta x_{4j} = 3 - x_{4j}(t)$. Proceed next to evaluate $\wedge x_{i+1}$.

For the $\wedge u_j$, the explanation of this ritual is straightforward. Step (1) tells us to decrease u_j by an arbitrary amount k_j if, for a "small" change in u_j alone, the effect will be to decrease ϕ. Similarly, there is to be an increase in u_j if, for a "small" increase, ϕ would decrease. Step (2) prevents u_j from becoming negative.

For the Δx_i, the justification is more tortuous. (Steps (3) and (4) are the obvious ones - respectively, lower and upper limits on the individual x_i.) As with the Δu_j, the sign of $\dfrac{\partial \phi (t)}{\partial x_i (t)}$ is primarily the criterion that determines whether to take a positive or a negative step. [1]

Preliminary hand calculations indicated, however, that the unqualified "direction of ascent (descent) rule" would lead to major oscillations during the process of convergence. For that reason, rule (1) -- a relaxation-type principle -- was inserted. Translated into English, the statement reads, "If one of the restraints is being violated, and if the direction-of-ascent rule would lead to an even greater violation of this restraint, then the particular x_i should not be changed." An IBM run is now in process for purposes of comparing the efficiency of the relaxation-type algorithm with that of the unmodified direction-of-ascent operation. [2]

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[1] The reader should note that ϕ is being minimized with respect to $\underline{u}$, and maximized with respect to $\underline{x}$.

[2] Since the original draft of this manuscript, the run has been completed. At the end of 110 steps, there was still no evidence of convergence.

Parameter values and initial conditions were identical with those for run 6. The only difference was the elimination of step (1) for the computation of Δx_i. For the reader's convenience, the time series on three of the variables are indicated below:

t	$x_{31}(t)$	$x_{22}(t)$	$u_1(t)$
0	1,428.6	571.4	12.10
10	1,368.6	651.4	11.90
20	1,128.6	451.4	11.50
30	1,428.6	611.4	11.90
40	1,128.6	531.4	11.90
50	1,308.6	651.4	11.50
60	1,165.6	651.4	11.90
70	1,248.6	491.4	11.30
80	1,309.6	651.4	12.30
90	1,008.6	531.4	11.70
100	1,308.6	731.4	11.70
110	1,068.6	651.4	11.70

Table 1. Parameters for Six Sets of Calculations

Run Number	1		2	3	4	5	6
	Steps 1-149	Steps 150-346					
P_1	12.00	12.00	12.00	12.00	12.00	11.60	12.00
P_3	0.23	0.23	0.23	0.23	0.23	0.23	0.60
q_2	1,000.	1,000.	1,000.	500.	300.	1,000.	1,000.
r_{c1}	10.	10.	10.	20.	20.	20.	20.
r_{c2}	10.	10.	10.	20.	20.	20.	20.
r_{21}	56.	56.	0	30.	30.	30.	30.
k_{11}	0.12	0.06	0.06	0.03	0.03	0.03	0.03
k_{12}	10.	10.	10.	20.	20.	20.	20.
k_{22}	10.	40.	10.	20.	20.	20.	20.
k_{22}	56.	56.	0	30.	30.	30.	30.
k_{12}	0.12	0.06	0.06	0.03	0.03	0.03	0.03
k_3	0.60	0.15	0.15	0.10	0.10	0.10	0.10
k_2	0.18	0.15	0.15	0.10	0.10	0.10	0.10
k_3	0.006	0.003	0.003	0.003	0.003	0.003	0.003
k_4	0.006	0.003	0.003	0.003	0.003	0.003	0.003

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At the present time, I am in an unpleasant quandary concerning the logic of these computational techniques. On the one hand, I have been unable to prove the necessity of convergence for either the modified or the unmodified procedure. On the other, I have been unable to construct a counter-example for a case where the k_i and the k_j may be made arbitrarily small. Even worse, there is not yet any general criterion for determining whether the relaxation-type procedure increases or decreases the efficiency in computing out a particular numerical example. These are all problems on which I will welcome mathematical advice.

5. Six computation runs

During the course of six IBM runs, the only numerical parameters altered were: p_1, p_3, q_1, the k_i and the k_j. The individual values for these are listed below in Table 1. The remainder were maintained at the values indicated in Appendix I.

In order to provide the most severe test of the computational procedure, the first run was made with a distinctly non-optimal initial position — in fact, from the zero vector for all x_i. (Exact numerical values for the $x(0)$ and $u(0)$ of each run are listed in Appendix II.) This non-optimal feature shows up in the time series for the first 20 steps (Figures 3-7). Most of the x_i indicate a strong upward trend during this initial phase. The only legitimate inference that can be drawn from the series at step (20) is that nothing like a stationary equilibrium has been reached. In fact, there continued to be significant trends in the x_i until 200-300 iterations had been performed. The process was finally stopped at the 346th step. The series for steps 327-346 are reproduced as Figures 9-12, and the vector at this point is given in Column A of Table 2.

Even at the 346th step, the system is not at a saddle point. According to the graphical solution (column C), at the optimum point $x_{11} = x_{12} = x_{22} = x_{32} = 0$. Although the IBM tabulation does indicate zero levels for x_{12} and x_{32}, nevertheless, x_{11} and x_{22} both show up at low positive levels.

More serious, the exact solution is infeasible. For example, the schedule requires more of stock 2 than is available -- 1,026.4 gallons, as against the 1,000 gallon limit. Only a simple adjustment is required, though, in order to obtain feasibility. The entries for x_{11}, x_{21}, x_{31}, and x_{22} were each multiplied by $\frac{1,000.0}{1,026.4} = 0.97428$. In order to satisfy f_3, it was necessary to make a slight increase in x_{41}; f_4 could be satisfied with a lower value of x_{42}. Finally, it was noted that the adjustment to the x_1 left 43.6 gallons of stock 1 in excess. Since stock 1 can be sold as premium grade gasoline by adding only 0.80 ml. of lead, this 43.6 gallon excess was credited to profits at a value of 11.816 ¢/gallon. The adjusted blending schedule is both feasible and efficient. The payoff, $g(x)$, amounts to \$230.58 as against a possible \$231.03, indicated by the graphical solution. These two numbers coincide to within 1 part in 500 -- well within the limits of accuracy of the graphical method.

Having established the general convergent nature of the algorithm, the remaining calculations were carried out from initial vectors that were considered to be sensible starting points. Run 2 was started off from C., the vector that is labelled "graphical solution" in Table 2. The solution never departed markedly from the initial values, and was halted at the 63rd step, giving a second column labelled "A., raw vector" in Table 2. The rough solution was adjusted in the same way as has been described for run 1, and the results also entered in Table 2. The adjusted $g(x)$ -- \$228.62 -- is again acceptably close to that for the graphical solution, \$228.73.
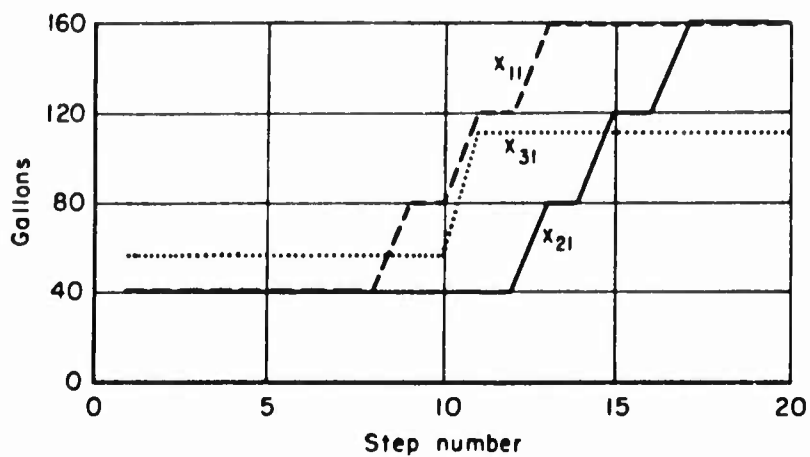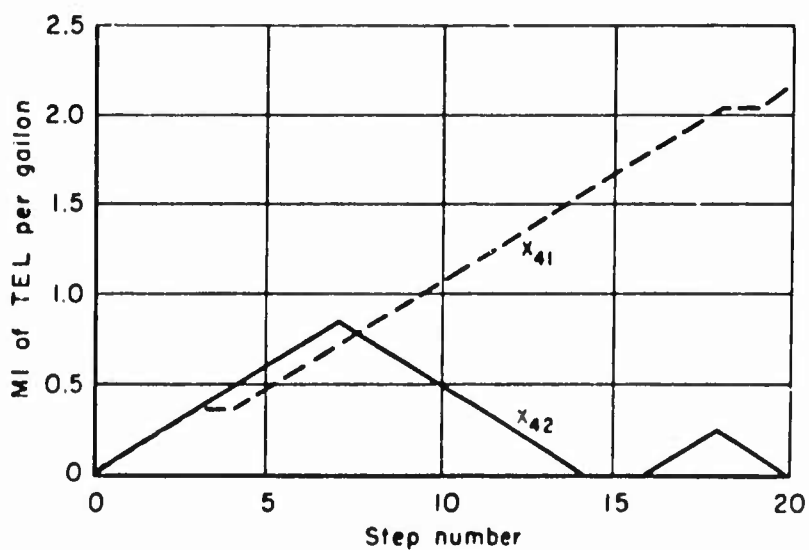
Fig. 3 — Steps 1-20 of run number 1

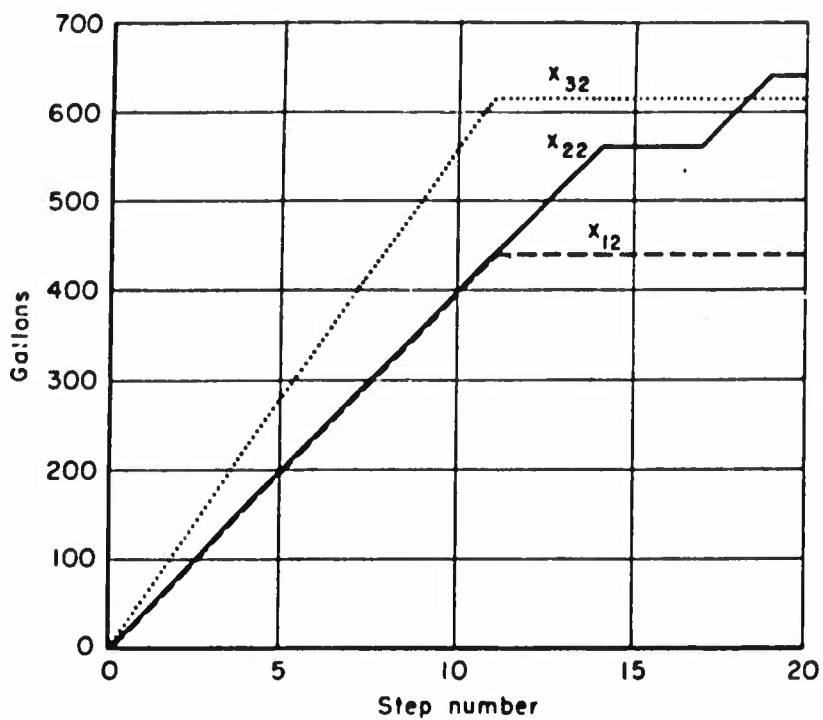Fig. 4 — Steps 1-20 of run number 1

Fig. 5 — Steps 1-20 of run number 1
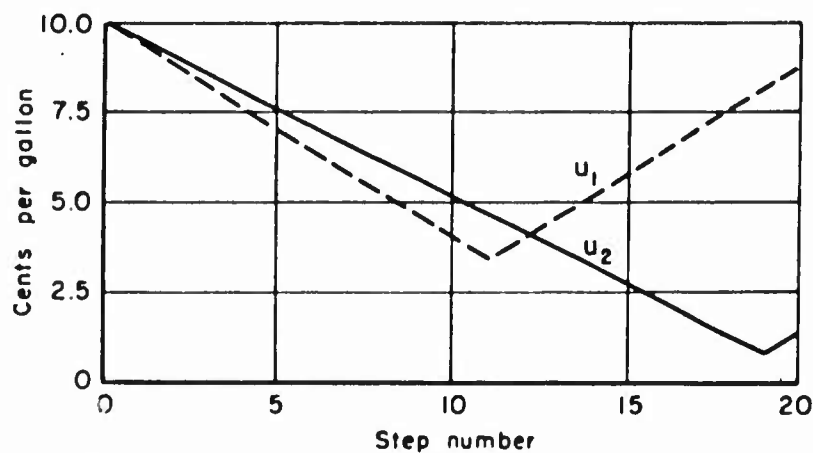

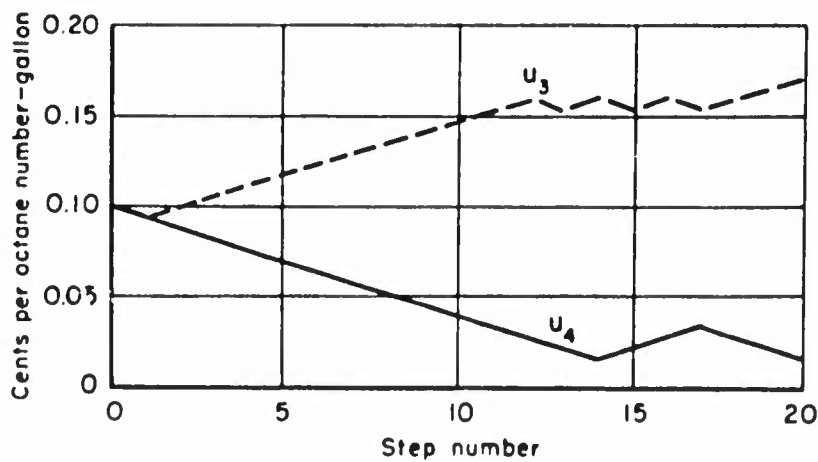Fig. 6 — Steps 1-20 of run number 1
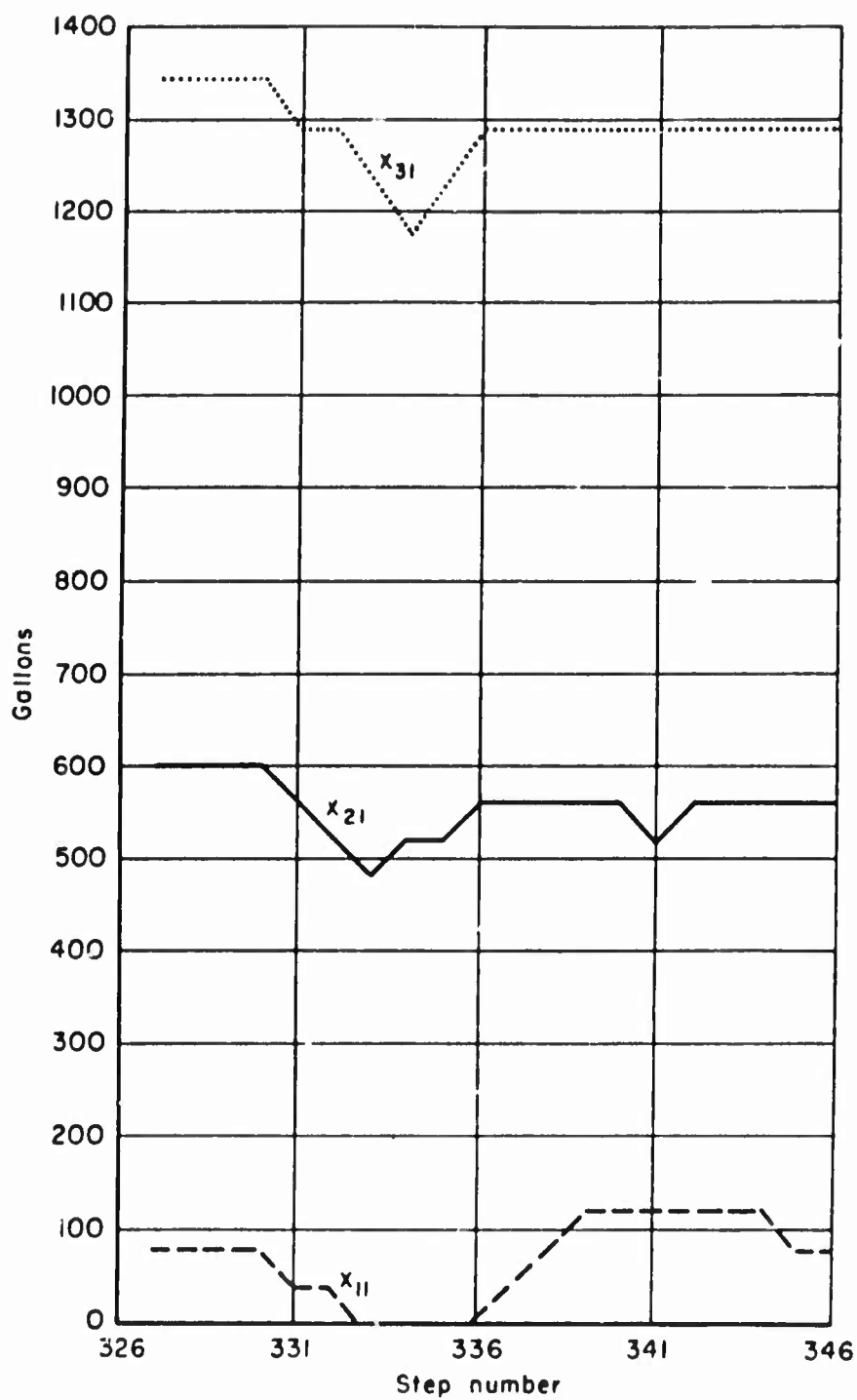

Fig. 7 — Steps 1-20 of run number 1
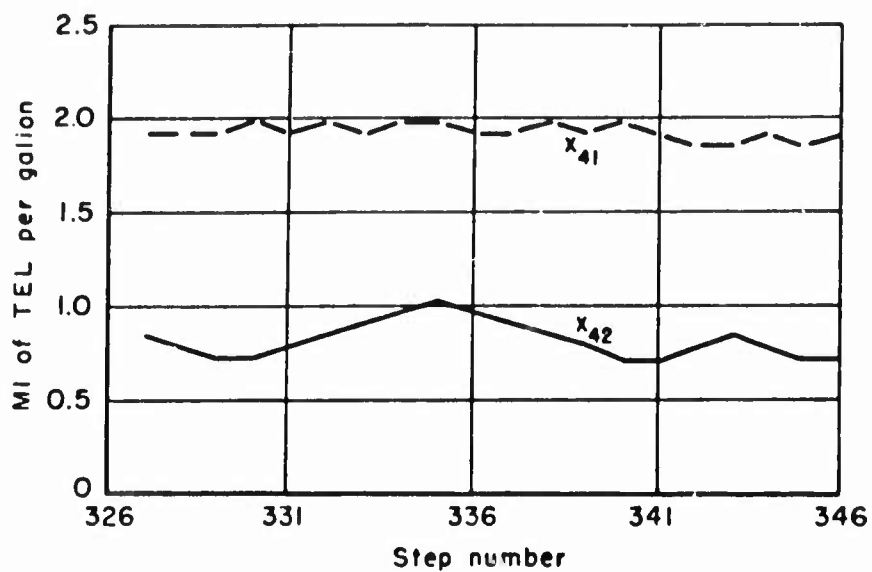
Fig. 8—Final 20 steps of run number 1

Fig. 9—Final 20 steps of run number 1

Fig. 10—Final 20 steps of run number 1

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Fig. 11—Final 20 steps of run number 1

Fig. 12—Final 20 steps of run number 1

Table 2. Solution Vectors, Runs 1 and 2

	Run 1			Run 2		
	A. Raw Vector	B. Adjusted Vector	C. Graphic Solution	A. Raw Vector	B. Adjusted Vector	C. Graphic Solution
Final t	346	--	--	63	--	--
x_{11}	80	77.9	0	960	960	1,000
x_{21}	560	545.6	571.4	920	920	1,000
x_{31}	1,298	1,254.9	1,429.6	0	0	0
$x_{.1}$	1.92	1.95	1.95	2.38	2.40	2.45
x_{12}	0	0	0	0	0	0
x_{22}	80	77.9	0	80	80	0
x_{32}	0	0	0	0	0	0
$x_{.2}$	0.72	0.70	0	0.84	0.70	0
$f_1(x)$	--	43.6	--	--	40.0	--
$f_2(x)$	--	0	--	--	0	--
$g(x)$ (dollars)	231.51	230.58	231.03	223.95	228.62	228.73

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Table 3. Solution Vectors, Runs 3 and 4

	Run 3			Run 4		
	$\underline{A}$ Raw Vector	$\underline{B}$ Adjusted Vector	$\underline{C}$ Graphic Solution	$\underline{A}$ Raw Vector	$\underline{B}$ Adjusted Vector	$\underline{C}$ Graphic Solution
Final t	70	--	--	30	--	--
x_{11}	0	0	0	0	0	0
x_{21}	705.7	691.9	716	531.4	473.4	542
x_{31}	711.3	700.3	714	428.6	428.6	428
x_{41}	2.79	2.80	2.75	3.0	3.0	3.00
x_{12}	0	0	0	0	0	0
x_{22}	100	98.0	70	380	400	230
x_{32}	0	0	0	0	0	0
x_{42}	0.75	0.70	0.70	0.79	0.70	0.70
$f_1(x)$	--	9.8	--	--	0	--
$f_2(x)$	--	0	--	--	0	--
$h(x)$ (dollars)	172.12	169.88	170.14	149.69	145.15	145.48

Table 4. Solution Vectors, Runs 5 and 6

	Run 5			Run 6		
	A Raw Vector	B Adjusted Vector	C Graphic Solution	A Raw Vector	B Adjusted Vector	C Graphic Solution
Final t	80	--	--	80	--	--
x_{11}	240	233.0	227	80	78.6	156
x_{21}	40	38.3	0	0	0	0
x_{31}	1,068.6	1,037.5	1,090	1,158.6	1,139.2	1,134
x_{41}	1.05	1.15	1.05	1.02	1.05	1.10
x_{12}	0	0	0	0	0	0
x_{22}	591.4	574.4	673	611.4	601.2	638.3
x_{32}	60	58.2	0	180	177.0	21.7
x_{42}	0.55	0.58	0.70	0.46	0.50	0.66
$f_1(x)$	--	0	--	--	0	--
$f_2(x)$	--	58.3	--	--	4.0	--
$f(x)$ (dollars)	224.01	223.45	222.67	225.92	222.15	221.94

2-1

During runs 1 and 2, the graphical solutions were determined in advance. For 3 - 6, however, they were obtained after the adjusted solution had been calculated. (For runs 3 and 4, the initial guess turned out to be the solution to the problem.) Tables 3 and 4 reveal that the algorithm continued to perform in a satisfactory way during the last four runs. For run 6, in fact, the adjusted solution at step 30 indicates a higher net realization than the graphical technique -- 2222.15, as against $221.94.

6. Interpretation of results

The numerical parameters used in run 1 for p_1, p_3, and q_1 were considered to be the basic set, and in each subsequent run not more than one of these was altered. In #3 and #4, the value of q_1 was changed; in run 5, p_1; and in run 6, p_3. The adjusted results for all the six runs are summarized by Table 5 in terms of four indicators -- the output of premium grade gasoline, the output of regular grade, the input of TEL, and the refinery realization. These data are also presented on Charts 13-16.

Run 2 differed from #1 in only one significant respect. During it, the refiner was not permitted to make stock 3 -- the fictitious intermediate product. The initial blending materials had to be assigned directly to the finished products. In other words, the refiner was not permitted to take full advantage of the concave octane number blending relationship.

This additional restriction had no effect upon the general strategy of converting virtually the entire volume of blending materials into premium grade gasoline. The restriction does have the effect of increasing the TEL requirements, and of decreasing the refiner's net realization.

The difference in realization at first glance appears small -- $229.6?, as against $230.58 in run 1. However, for a refinery turning out 20,000 barrels of gasoline per calendar day, such a discrepancy would come to an annual figure of roughly $300,000! To put the matter another way, the first blending schedule does the same job as the second, with a total TEL requirement that is about 20% smaller. From this, I would conclude that it is eminently worthwhile for a refiner to incur considerable expense in testing gasoline blends, and in attempting to predict the occurrence of curvilinear octane relationships.

In the first run, it turned out that the most profitable blending schedule was one that assigned all ?,?00 gallons into premium grade gasoline. This result was quite in line with a rule-of-thumb that is commonly heard among refiners -- to wit, that the maximum profits will be obtained by making the maximum amount of the high-priced product.[1] This rule-of-thumb is not shaken by the results of run 3 or 4. At a q_1 availability level of 500 gallons, the best strategy is to produce virtually nothing but premium grade gasoline. At a q_1 level of 300 gallons, however, the 3.0 ml. limit on TEL concentration has come into effect. At this low q_1 level, the best the refiner can do is to add 3.0 ml. to each gallon of premium grade gasoline, and and to assign the left-over stock 2 to the production of the regular grade product.

The preceding results do not speak well for an alternatively-heard dictum -- that the best general course to follow is to assign 3.0 ml. of ethyl fluid

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[1] I do not allege that refiners generally follow such a rule -- only that they _say_ they do.

Table 5. Summary of Runs 1 - 6, Adjusted Data

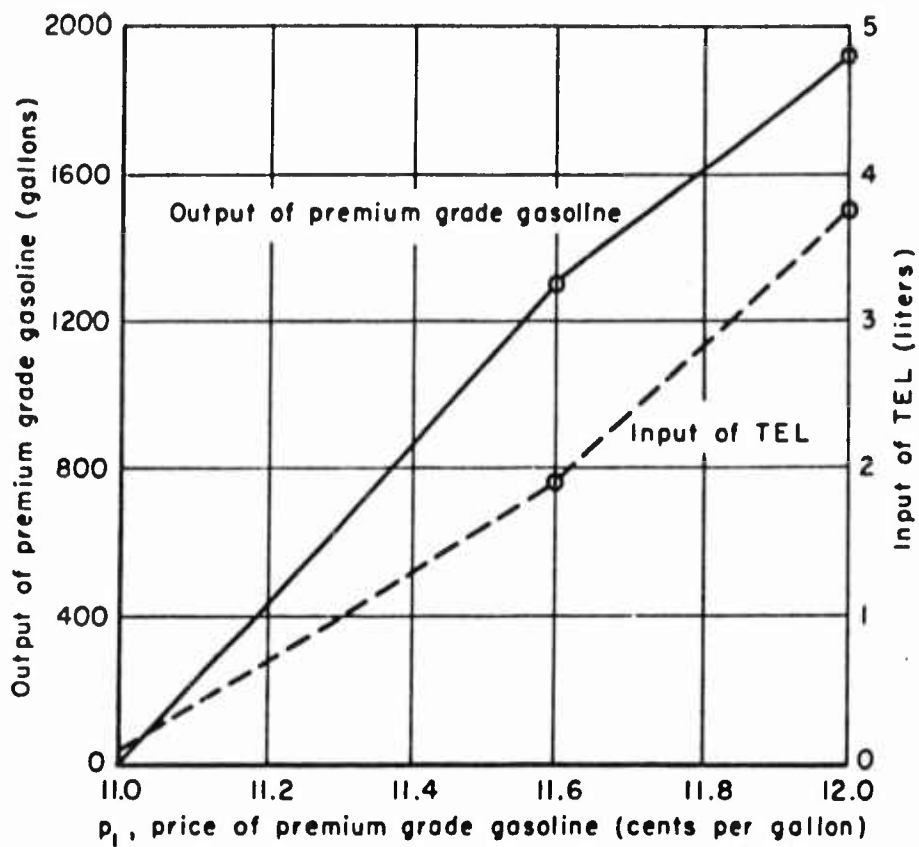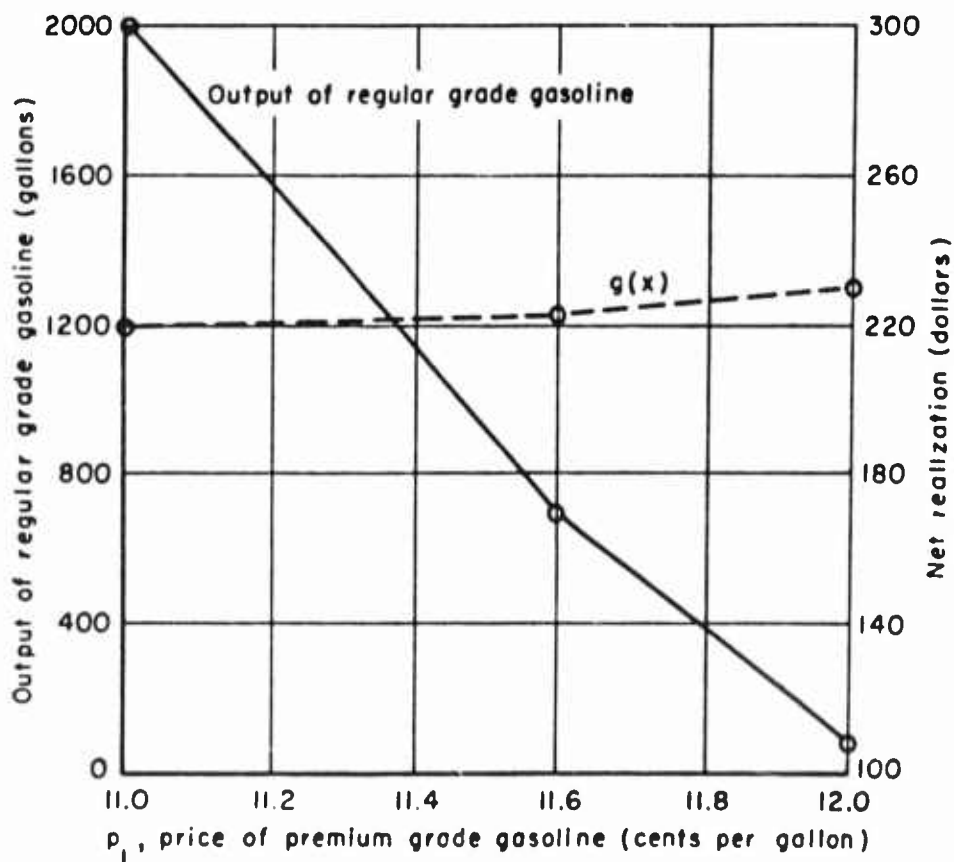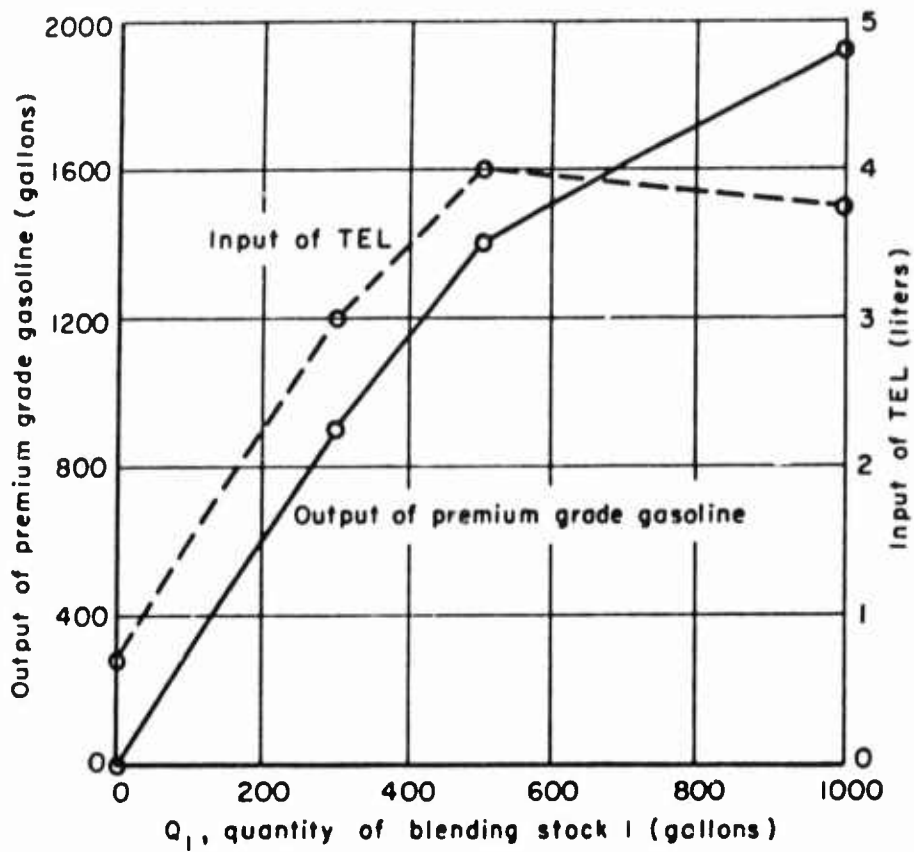| Run Number:	1	2	3	4	5	6
x_1	1,000	2,000	500	200	1,000	2,000
F_1	12	12	12	12	11.6	12
P_3	.23	.23	.23	.25	.23	.60
Output of premium gasoline (gallons)	1,922.0	1,920.0	1,452.0	930.0	1,309.3	1,211.2
Output of regular gasoline (gallons)	77.9	80.0	98.0	103.0	690.7	782.2
Input of TEL (liters)	3.752	4.600	3.975	2.950	1.913	1.671
F(x) (dollars)	230.58	228.62	169.88	145.15	223.45	222.35

Fig. 13
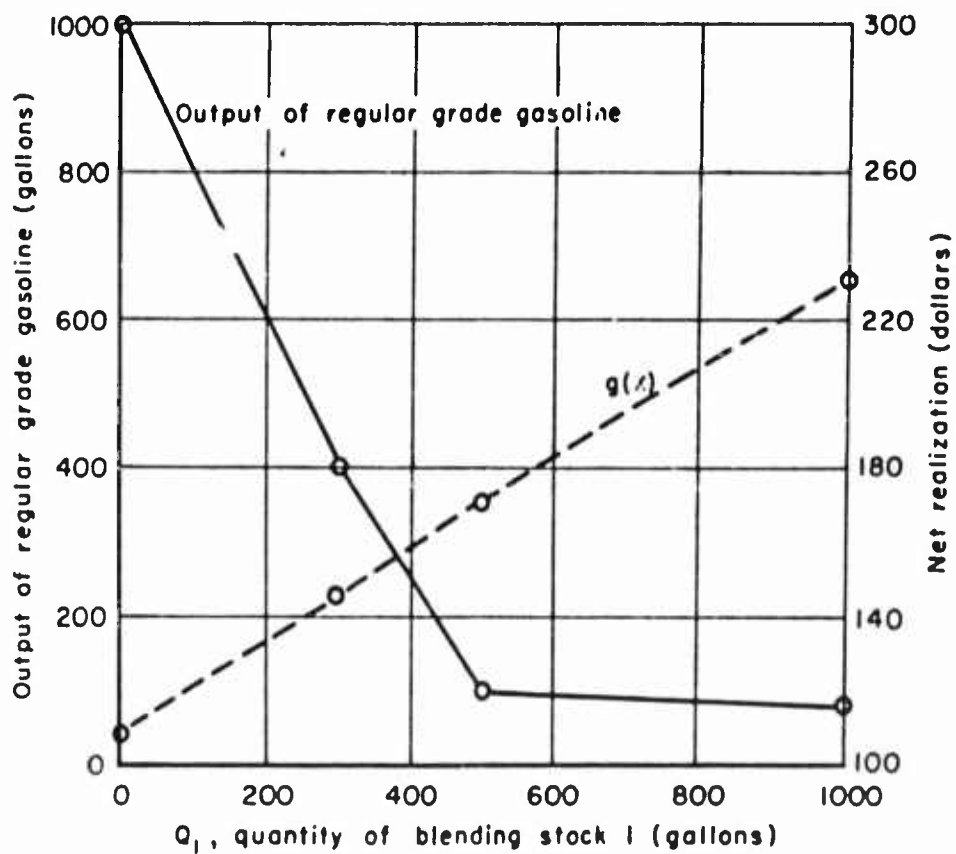

Fig. 14

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Fig. 15

Fig. 16

to each gallon of product. Only in making premium grade gasoline during
run 3 did it pay to use the maximum allowable TEL concentration.

Runs 5 and 6 cast doubt, not only on the 3.0 ml. principle, but also
on the maximum-production-of-premium theory. In run 5, the only para-
meter change from #1 was a reduction in the price of premium grade
product from 12¢/gallon to 11.6¢. This difference in the price structure
is sufficient to bring about a substantial increase in the optimal out-
put of regular grade product -- from less than 100 gallons in #1, to
almost 700 gallons in #5. This shift is also accompanied by a marked
reduction in the total input of ethyl fluid.

For run 6, a different sort of change in the price structure was
tried. The price of ethyl fluid was virtually trebled -- from 0.23¢/ml.
to 0.60¢. Again comparing the results with #1, there is a shift into
the production of regular grade gasoline, and a reduction in the input
of ethyl fluid.

To put the matter another way, the rules-of-thumb imply that the
same input and output relationships are optimal under all price struc-
tures. One of these rules does happen to give a good performance for
a particular current set of prices, but does not apply outside this
limited range. Unfortunately, there is no easy escape. The only way
to verify one of these rules-of-thumb in a concrete case is to carry
through a detailed formal analysis.

7. Conclusions

At this point, it is appropriate to sum up the findings. On the
negative side, the study has demonstrated that certain rules-of-thumb
work badly -- even though these principles have occasionally been put
forward by men in the refining industry. The study, moreover, has shown

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that the optimal input and output relationships will be intimately linked with the price structure. Figures 13 and 14 give some clues as to the nature of this linkage. Before the economist jumps to the conclusion that these really _are_ supply and demand curves, however, he is urged to reread the caveats of Section 3.

On the positive side, the claims are necessarily more cautious. The study indicates that a refiner will do well to make a careful investigation of his gasoline stocks for non-linear blending characteristics. The results do _not_ imply that a 20% saving in TEL costs will inevitably occur.

More significant from a long-range viewpoint, the computing runs indicate that it is possible to solve concave programming problems on a digital computer. The particular procedure employed is undoubtedly wasteful of machine time, and superior methods will surely evolve. The next programming problem that will be attacked is one that has been formulated by one of the major West Coast refiners. Although this coming problem has 22 x_i and 8 u_j, the basic notion is the same. The quantities available of various blending stocks will be taken for granted, and the analysis carried on from that point. Certain cutting temperatures will also enter as independent variables. At a later date, it is expected that the model will be expanded to incorporate such process variables as reactor temperatures and recycle ratios.

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9. U. S. Bureau of Mines, Petroleum Refineries, Including Cracking Plants, in the United States, January 1, 1952, Information Circular 7646, September, 1952.

Appendix I. Constants for Six Sets of Calculations

Sources:

$p_1 = 12¢/gal.$)
)
)
$N_1 = 90$ octane)
number)
)

Ref. 8 gives the following Gulf Coast, bulk cargoes price range for 90 octane (ASTM Research) premium motor gasoline: 11.75 - 12 - 12.25¢/gal. These prices were in effect on November 24, 1952.

$p_2 = 11¢/gal.$)
)
)
$N_2 = 83$ octane)
number)
)

Ref. 8 gives the following Gulf Coast, bulk cargoes price range for 83 octane (ASTM Research) regular motor gasoline: 10.75 - 11 - 11.25¢/gal. These prices were in effect on November 24, 1952.

$p_3 = 0.23¢/ml.$ of)
TEL)
)

The Los Angeles Sales Office of the Ethyl Corporation gave this quotation on November 21, 1952. It applies to motor mix ethyl fluid, delivered in tank-car lots to any U. S. destination.

$q_1 = 300, 500, 1,000$ gal.)
of catalytic-cracked-)
plus-polymer gasoline)
)
$q_2 = 1,000$ gal. of thermal)
cracked gasoline)
)

Ref. 9, p. 5 indicates the following break-down of U. S. cracking plant capacity as of January 1, 1952:

thermal cracked: 724,690 barrels/day; catalytic cracked gasoline: 407,544 barrels/day.

N.B. There are wide variations in the ratio of thermal to catalytic capacity as between individual refineries and refining regions.

Appendix I. (continued)

The a_i, b_i, and c_i coefficients for each stock were derived from the Bogen and Nichols data [1, Table II, p. 2630]. The three sets of observations are shown on Figure 1. The individual coefficients had the following numerical values:

Stock #	1	2	3
a_i	9L.8	89.6	9L.1
b_i	.233	.L33	.266
c_i	-8.931	-12.13	-9.06

Appendix II. Initial Vectors for Six Sets of Calculations

..un Number	1	2	3	4	5	6
$x_{11}(0)$	0	1,000.0	0	0	0	0
$x_{21}(0)$	0	1,000.0	785.7	471.4	0	0
$x_{31}(0)$	0	0	714.3	1,428.6	1,428.6	1,428.6
$x_{41}(0)$	0	2.50	2.0	3.0	1.2	1.2
$x_{12}(0)$	0	0	0	0	0	0
$x_{22}(0)$	0	0	0	400.0	571.4	571.4
$x_{32}(0)$	0	0	0	0	0	0
$x_{42}(0)$	0	0	0	0.7	0.7	0.7
$u_1(0)$	12.00	12.10	12.10	12.00	12.10	12.10
$u_2(0)$	12.00	10.75	10.75	11.00	10.75	10.75
$u_3(0)$	0.100	0.154	0.154	0.214	0.154	0.154
$u_4(0)$	0.100	0.003	0.154	0.052	0.154	0.154

Addendum to P-383, "Concave Programming for Gasoline Blends"

In discussing P-383, Dr. Martin Beckman uncovered a problem to which I had not previously given attention. He has made the point that for a function of many variables, $f(x)$, to be truly concave, it is necessary but <u>not</u> sufficient for that function to be concave in <u>each variable taken separately</u>.

The basic problem arises out of the fact that the function xy is neither concave nor convex - for nonnegative independent variables x and y. This is despite the fact that it is concave <u>and</u> convex in either variable separately.

Proof: Consider two points (x_1, y_1) and (x_2, y_2). Convexity would require:

$$(1) \quad \left[\frac{x_1 + x_2}{2} \right] \left[\frac{y_1 + y_2}{2} \right] \leq \frac{1}{2} x_1 y_1 + \frac{1}{2} x_2 y_2$$

$$\left[x_1 + x_2 \right] \left[y_1 + y_2 \right] \leq 2 x_1 y_1 + 2 x_2 y_2$$

$$x_1 y_2 + x_2 y_1 \leq x_1 y_1 + x_2 y_2$$

$$(2) \quad x_1 (y_2 - y_1) \leq x_2 (y_2 - y_1)$$

For nonnegative x and y, and for $y_2 > y_1$, expression (2) requires $x_1 \leq x_2$. But the convexity condition applies to any arbitrary (x_1, y_1) and (x_2, y_2). This is a contradiction. Similarly for concavity. Q.E.D.

Now, what are the implications of this result for the gasoline blending model? Fortunately, it turns out that by a re-definition of variables, the pay-off function $g(x)$ can be made concave -- indeed linear. Unfortunately, though, this re-definition does not lead to any rigorous proof of the concavity of restraint

equations (9) and (10). On the contrary, it shows up the possibility of non-concavity in these restraint conditions when two of the blending stocks have widely divergent lead susceptibilities.

Let us define new variables, x_{51} and x_{52}, in the following way:

$$x_{51} = x_{41}(x_{11} + x_{21} + x_{31})$$

$$x_{52} = x_{42}(x_{12} + x_{22} + x_{32})$$

Equation (3) can now be transformed into a linear form involving the two new variables, x_{51} and x_{52} :

$$(3a) \quad g(x) = p_1 (x_{11} + x_{21} + x_{31}) + p_2 (x_{12} + x_{22} + x_{32}) - p_3(x_{51} + x_{52})$$

To simplify the discussion of equations (9) and (10), I shall arbitrarily assume that both x_{31} and x_{32} are constrained to be zero, and will focus attention on the function $f_3 (x)$, dealing with the octane specification of the premium grade gasoline. Suppose that the octane numbers and the quantities available of the two blending stocks had been as follows:

	Stock 1	Stock 2
Quantity available, x_{11}	1,000 gal.	1,000 gal.
Octane number, clear	4.0	90.0
Octane number, with 3 ml. of TEL	0.0	94.8
Number of ml./gal. required for 90 octane leaded gasoline, x_{41}	3.0	0
Total number of ml. required for 90 octane leaded gasoline, x_{51}	3,000	0

Assuming straight line interpolation at constant lead levels for the two stocks, and assuming a 50-50 blend, we come up with these results for the blend:

Quantity available, $(x_{11} + x_{21})$	2,000 gal.
Octane number, clear	82.0
Octane number, with 3 ml. of TEL	92.4
Number of ml./gal. required for 90 octane leaded gasoline, x_{41}	1.6
Total number of ml. required for 90 octane leaded gasoline, x_{51}	3,200

In other words, if the two initial materials are ethylized and marketed separately, the average TEL requirement per gallon comes to 1.5 ml. If the two are blended together, the same amount of premium gasoline is produced, but the average lead requirement increases to 1.6 ml. This behavior clearly violates concavity of the function $f_3 (x_{11}, x_{21}, x_{31}, x_{51})$, and leads to the possibility of multiple isolated maxima. Lacking the concavity property in our functions, we may be led to adopt blending schedules that are locally optimal, but which do not, in fact, represent the best of all solutions available.

Now, how serious are the possibilities of such local maxima? The problem cannot be shrugged off, but I believe that in most particular applications these local extrema can be detected by the investigator. In order for the violation of concavity to take place, some of the blending material must be particularly high in lead susceptibility, and some of it must be extremely low. In addition, the first material must require a high TEL concentration in order to meet the specification, and the second a low TEL level. Knowing something about the occurrence of such pitfalls, the intelligent refiner should be able to avoid ensnarement.

The difficulties arising out of non-concavity are not unique to the programming method described in P-383. The same argument would apply if

x_{41} and x_{42} were taken as parameters, and a separate linear programming problem then run off for each of many combinations of the two. This difficulty would arise in the case of any trial-and-error method that consisted in changing one variable at a time, and observing the effects upon the payoff, $g(x)$. And finally, such failure of the proper curvature conditions could frustrate an optimization via a Lange-Lerner shadow price market mechanism.

The dilemma raised by Dr. Beckman should not be viewed as an absolute impasse, but rather as a challenge to the ingenuity of workers in this field. These latter can take comfort in recalling that truly rigorous analysis is seldom applicable within the domain of applied mathematics.

<u>ERRATA</u>

Mr. Lloyd Philipson has pointed out the following misprints:

last line of p. 12 should read: "If $u_j(t) + \Delta u_j \geq 0$, then $\Delta u_j = \widehat{\Delta u_j}(t)$"

line 6 of p. 13 should read: "If $\dfrac{\partial \phi(t)}{\partial x_1(t)} < 0$, then the 'candidate'

$\widehat{\Delta x_1} = -k_1$"